

UNIVERSIDAD NACIONAL DE CÓRDOBA
Instituto Multidisciplinario de Biología Vegetal

Av. Vélez Sarsfield 299, 2° piso. 5000 Córdoba, Argentina. Dirección postal: Casilla de Correo 495.
5000 Córdoba, Argentina
Telefax: (54) 351-433 4141 / secretaria@imbiv.unc.edu.ar / http://imbiv.unc.edu.ar



ESTUDIO:	*ANALISIS POR GCMS*	FECHA	31/10/2014

SOLICITANTE:	**Ing. Daniel Yorio**
No. de registro/solicitud:	**28_2014**
Análisis requerido:	**Identificación y cuantificación de compuestos presentes en las muestras**
Muestras:	**Muestra A1, A2, A3, F1, F2 y F3**
Fecha de recepción	**29 de octubre de 2014**

Procesamiento de la muestra

Las muestras son cartucho para volátiles, y cada una se eluye con 1 ml de Sulfuro de Carbono.
Se agrego a cada muestra 0.1748 mg de timol como estándar interno (disuelto en CS2).

Equipo:

GCMS Clarus 600, Perkin Elmer N° de serie 664N9100105. Los datos fueron adquiridos empleando el programa Turbo-Mass 5.4.2.

Columna: DB5 (60 m, 0.25 mm ID, 0.25 μm de partícula), marca Perkin Elmer. Carrier: Helio (49.6 psi), Inyector: 250ºC. Programa: Temp inicial 40ºC (1 min), Rampa: 6ºC/min hasta 90ºC, rampa: 18ºC/min, Temp Final 180ºC. La muestra se inyectó en modo de inyección Splitless.

GC-MS El cromatograma fue obtenido en modo ‘‘scan´´, desde m/z =30 a m/z =400 (scan time: 0.2 s, inter-scan time: 0.1s), solvent delay: 1 min.

Resultados obtenidos:

La identificación de los picos se realiza por comparación con los espectros de las Bibliotecas del programa NIST MS Search 2.0.

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Tabla 1: Valores encontrados para la muestra A1.

	Tiempo de retención (min)	Mg de compuesto/ml	Identificación
1	2.704	4,0712	Name: METHANOL Formula: CH_4O MW: 32 CAS#: 67-56-1
2	2.759	0,5381	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3.134	35,3198	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	3.704	221,3225	Name: Pentane, 3-methyl- Formula: C_6H_{14} MW: 86 CAS#: 96-14-0
5	4.000	27,9575	Name: Pentane, 2,2-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 590-35-2
6	4.045	20,4519	Name: Pentane, 2,4-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 108-08-7
7	4.090	198,3110	Name: Cyclopentane, methyl- Formula: C_6H_{12} MW: 84 CAS#: 96-37-7
8	4.485	15,8549	Name: Cyclohexane Formula: C_6H_{12} MW: 84 CAS#: 110-82-
9	12.983	0,1748	Std

Tabla 2: Valores encontrados para la muestra A2.

	Tiempo de retención (min)	Mg de compuesto/ml	Identificación
1	2.689	0,5561	Name: METHANOL Formula: CH_4O MW: 32 CAS#: 67-56-1
2	2.744	0,0581	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3.124	2,0553	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	3.659	19,6864	Name: Pentane, 3-methyl- Formula: C_6H_{14} MW: 86 CAS#: 96-14-0
5	3.965	1,8758	Name: Pentane, 2,2-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 590-35-2
6	4.015	1,0112	Name: Pentane, 2,4-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 108-08-7
7	4.060	12,9350	Name: Cyclopentane, methyl- Formula: C_6H_{12} MW: 84 CAS#: 96-37-7
8	4.460	0,9566	Name: Cyclohexane Formula: C_6H_{12} MW: 84 CAS#: 110-82-
9	13.008	0,1748	Std

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Tabla 3: Valores encontrados para la muestra A3.

	Tpo de retención (min)	Mg compuesto/ mL	Identificacion
1	2,684	0,2298	Name: METHANOL Formula: CH_4O MW: 32 CAS#: 67-56-1
2	2,739	0,0735	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3,139	1,6462	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	4,090	0,1250	Name: Pentane, 2,2-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 590-35-2
5	4,135	0,1026	Name: Pentane, 2,4-dimethyl- Formula: C_7H_{16} MW: 100 CAS#: 108-08-7
6	4,175	0,8965	Name: Cyclopentane, methyl- Formula: C_6H_{12} MW: 84 CAS#: 96-37-7
7	4,565	0,0988	Name: Cyclohexane Formula: C_6H_{12} MW: 84 CAS#: 110-82-
8	12,978	0,1748	Std

Tabla 4: Valores encontrados para la muestra F1.

	Tpo de re-tención (min)	Mg com-puesto/ mL	Identificacion
1	2.689	0,0670	Name: METHANOL Formula: CH_4O MW: 32 CAS#: 67-56-1
2	2.744	0,0108	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3.119	0,4048	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	4.050	0,0103	Name: Cyclopentane, methyl- Formula: C_6H_{12} MW: 84 CAS#: 96-37-7
5	13.023	0,1748	Std

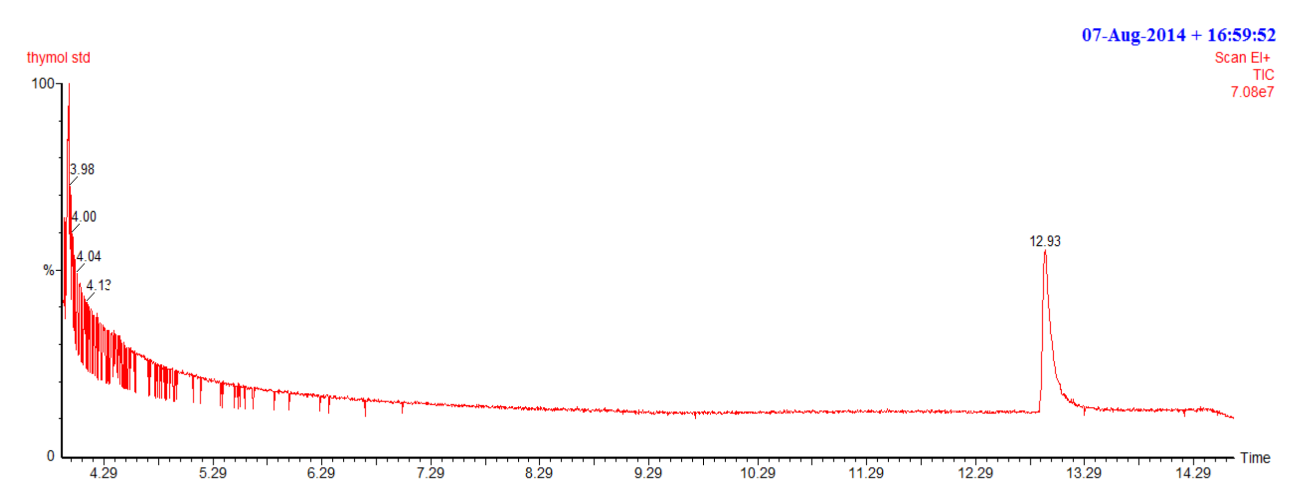
Tabla 5: Valores encontrados para la muestra F2.

	Tiempo de retención (min)	Mg com-puesto/ mL	Identificacion
1	2.749	0,0213	Name: ACETIC ACID, HYDROXY- Formula: $C_2H_4O_3$ MW: 76 CAS#: 79-14-1
2	2.804	0,0056	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3.184	0,2571	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	4.150	0,0049	Name: Cyclopentane, methyl- Formula: C_6H_{12} MW: 84 CAS#: 96-37-7
5	12.928	0,1748	Std

Tabla 6: Valores encontrados para la muestra F3.

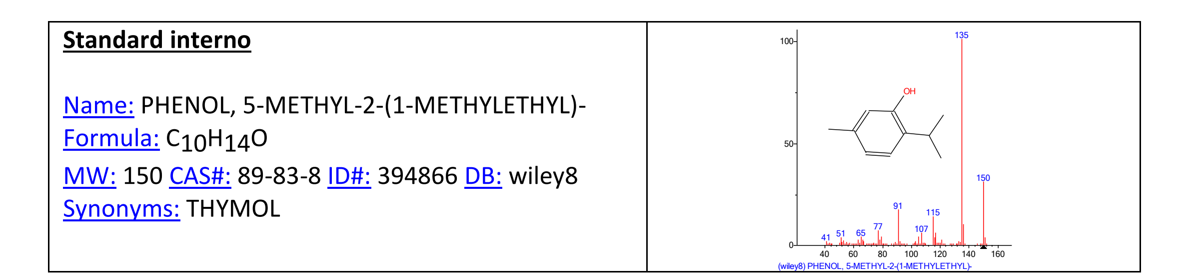
	Tiempo de retención (min)	Mg com-puesto/ mL	Identificacion
1	2.684	0,2268	Name: ACETIC ACID, HYDROXY- Formula: $C_2H_4O_3$ MW: 76 CAS#: 79-14-1
2	2.739	0,0211	Name: FORMIC ACID, METHYL ESTER Formula: $C_2H_4O_2$ MW: 60 CAS#: 107-31-3
3	3.119	1,5252	Name: Ethyl ether Formula: $C_4H_{10}O$ MW: 74 CAS#: 60-29-7
4	13.108	0,1748	STd

Espectro del compuesto de referencia (estándar interno) y perfil cromatográfico



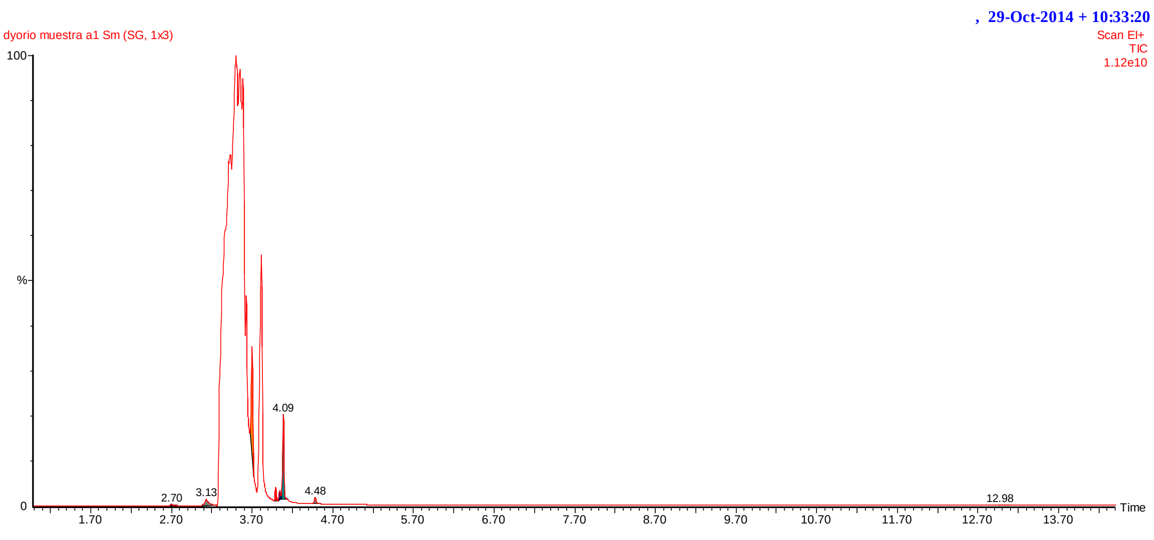
Standard interno

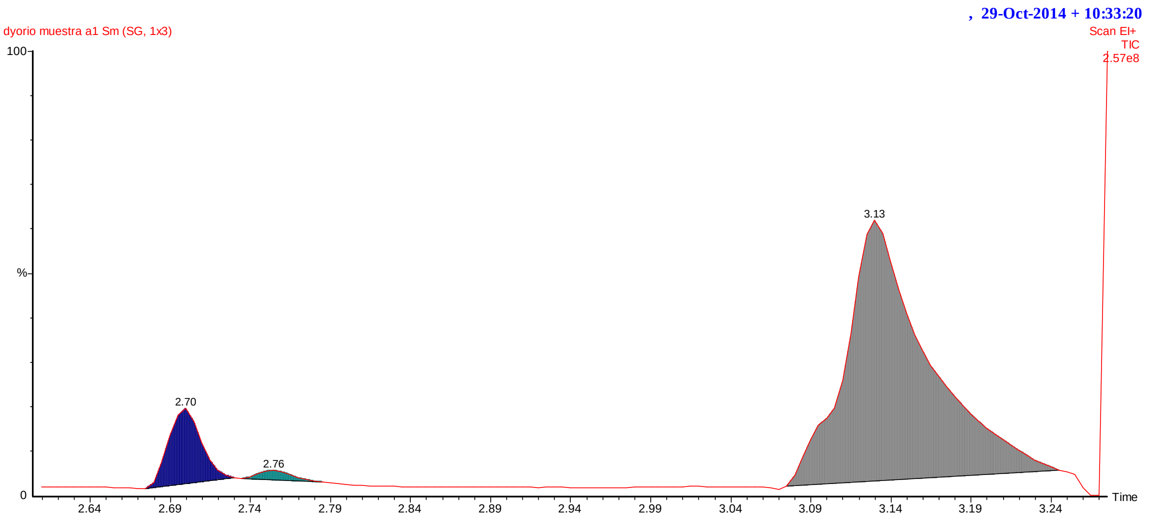
Name: PHENOL, 5-METHYL-2-(1-METHYLETHYL)-
Formula: $C_{10}H_{14}O$
MW: 150 CAS#: 89-83-8 ID#: 394866 DB: wiley8
Synonyms: THYMOL

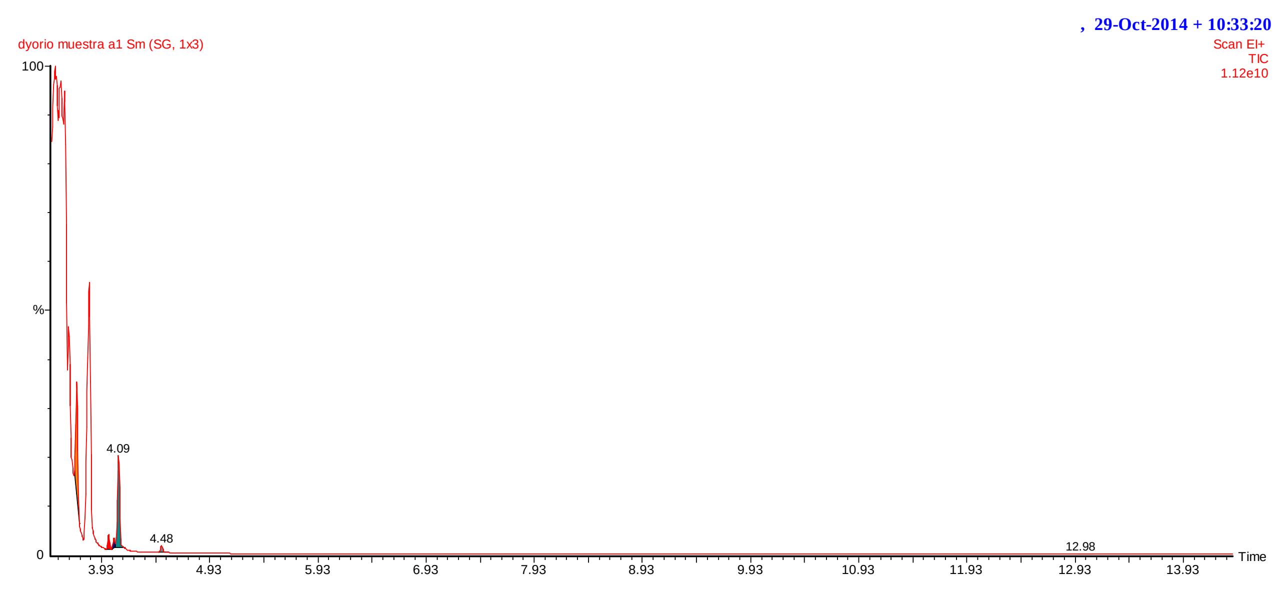




Perfil cromatográfico obtenido por CGMS para las muestras.





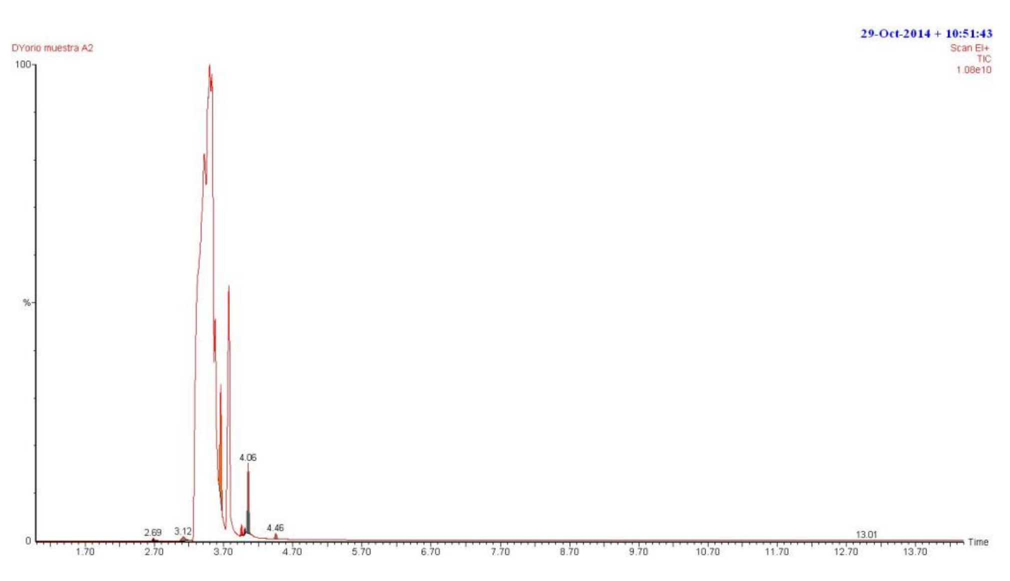


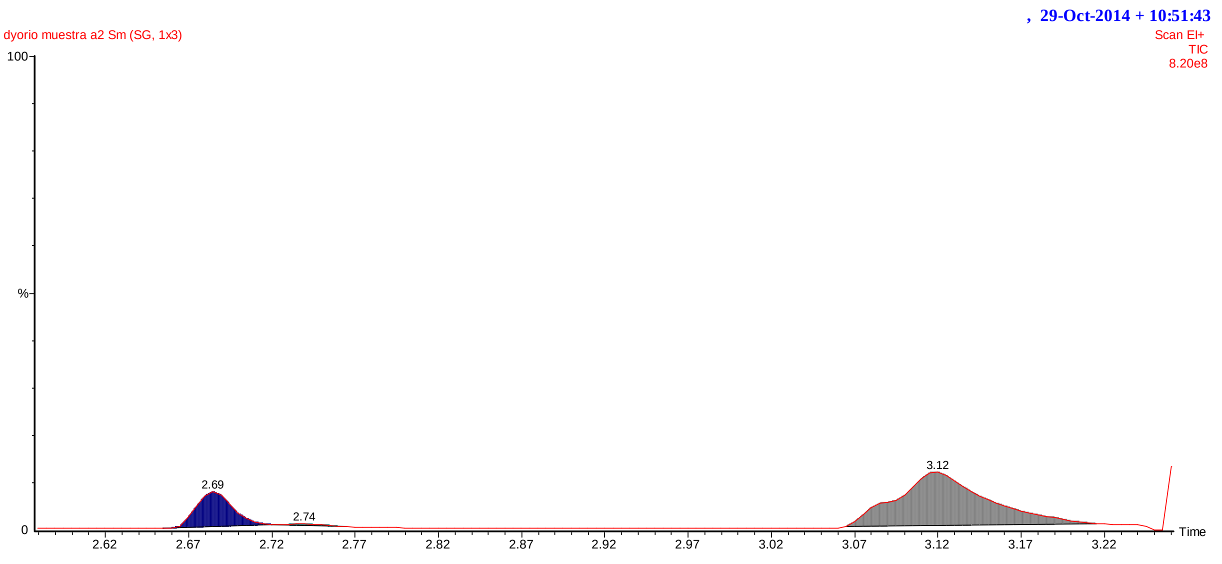
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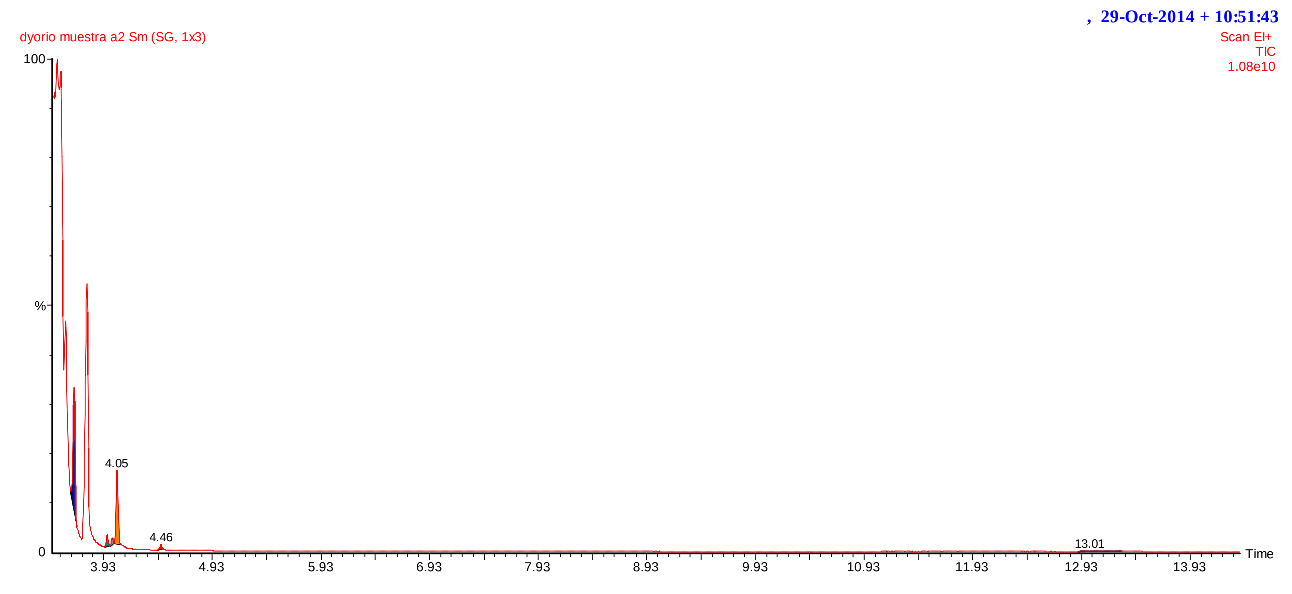
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DYorio muestra A3 NR+Sm (SG, 1x3)

, 29-Oct-2014 + 11:11:46
Scan EI+
TIC
1.18e10

100 % 0

2.68 3.14 4.17 4.56 12.99

1.70 2.70 3.70 4.70 5.70 6.70 7.70 8.70 9.70 10.70 11.70 12.70 13.70 Time

DYorio muestra A3 NR+Sm (SG, 1x3)

, 29-Oct-2014 + 11:11:46
Scan EI+
TIC
7.75e8

100 % 0

2.68 2.74 3.14

1.88 1.98 2.08 2.18 2.28 2.38 2.48 2.58 2.68 2.78 2.88 2.98 3.08 3.18 3.28 Time

dyorio muestra a3 Sm (SG, 1x3)

, 29-Oct-2014 + 11:11:46
Scan EI+
TIC
4.36e8

100 % 0

4.17 4.56 12.98

4.17 4.67 5.17 5.67 6.17 6.67 7.17 7.67 8.17 8.67 9.17 9.67 10.17 10.67 11.17 11.67 12.17 12.67 13.17 13.67 14.17 Time



dyorio muestra f1
, 29-Oct-2014 + 11:30:52
Scan EI+
TIC
1.21e10
100
%
0
3.69
3.56
3.51
3.47
3.43
3.73
1.70 2.70 3.70 4.70 5.70 6.70 7.70 8.70 9.70 10.70 11.70 12.70 13.70 Time

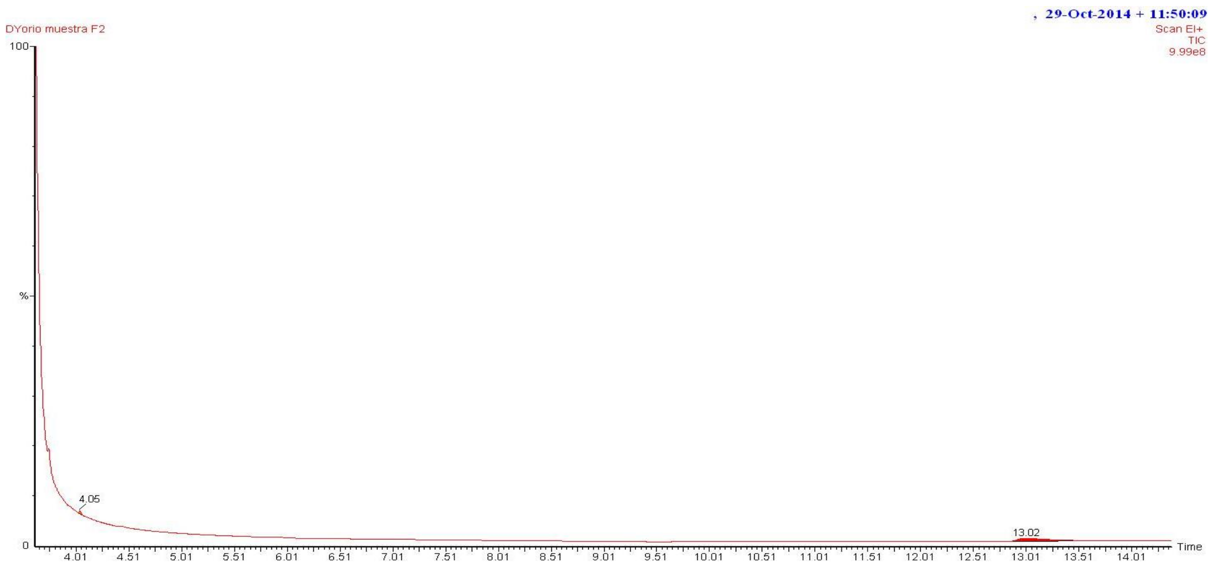
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29-Oct-2014 + 11:30:52
Scan EI+
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100
%
0
2.75 2.80
3.18
1.20 1.30 1.40 1.50 1.60 1.70 1.80 1.90 2.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 Time

DYorio muestra F1
29-Oct-2014 + 11:30:52
Scan EI+
TIC
8.00e8
100
%
0
4.15
12.93
4.09 4.59 5.09 5.59 6.09 6.59 7.09 7.59 8.09 8.59 9.09 9.59 10.09 10.59 11.09 11.59 12.09 12.59 13.09 13.59 14.09 Time



DYorio muestra F2
29-Oct-2014 + 11:50:09
Scan EI+
TIC
1.06e10
100
%
0
2.69
3.12
4.05
13.02
1.70 2.70 3.70 4.70 5.70 6.70 7.70 8.70 9.70 10.70 11.70 12.70 13.70
Time

DYorio muestra F2
29-Oct-2014 + 11:50:09
Scan EI+
TIC
9.40e7
100
%
0
3.12
2.69
2.74
2.25 2.30 2.35 2.40 2.45 2.50 2.55 2.60 2.65 2.70 2.75 2.80 2.85 2.90 2.95 3.00 3.05 3.10 3.15 3.20 3.25
Time





dyorio muestra f3

29-Oct-2014 + 12:09:10
Scan EI+
TIC
1.22e10

100 / % / 0
2.68 3.12 13.11
1.70 2.70 3.70 4.70 5.70 6.70 7.70 8.70 9.70 10.70 11.70 12.70 13.70 Time

dyorio muestra f3

, 29-Oct-2014 + 12:09:10
Scan EI+
TIC
1.37e9

100 / % / 0
2.68 2.74 3.12
1.57 1.67 1.77 1.87 1.97 2.07 2.17 2.27 2.37 2.47 2.57 2.67 2.77 2.87 2.97 3.07 3.17 3.27 3.37 3.47 3.57 Time

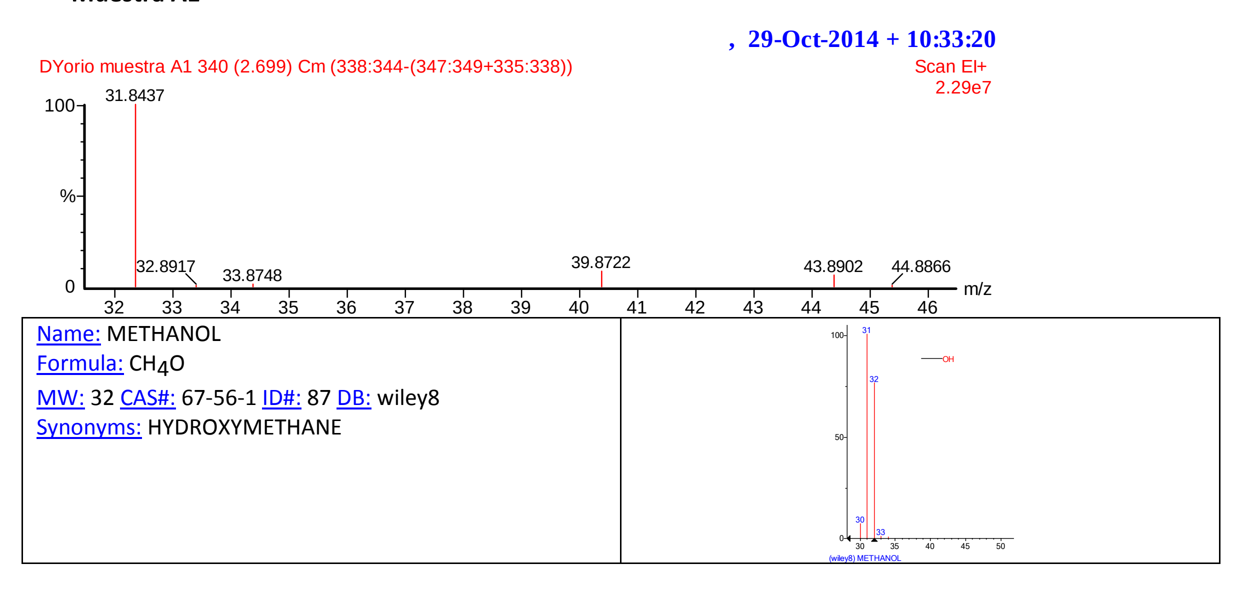
dyorio muestra f3

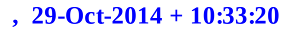
29-Oct-2014 + 12:09:10
Scan EI+
TIC
9.56e7

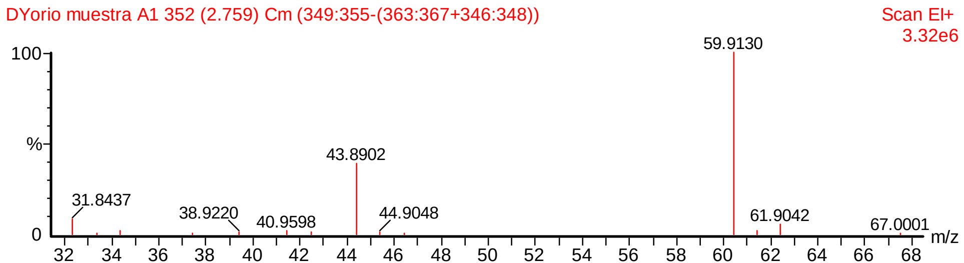
100 / % / 0
13.11
4.16 4.66 5.16 5.66 6.16 6.66 7.16 7.66 8.16 8.66 9.16 9.66 10.16 10.66 11.16 11.66 12.16 12.66 13.16 13.66 14.16 Time

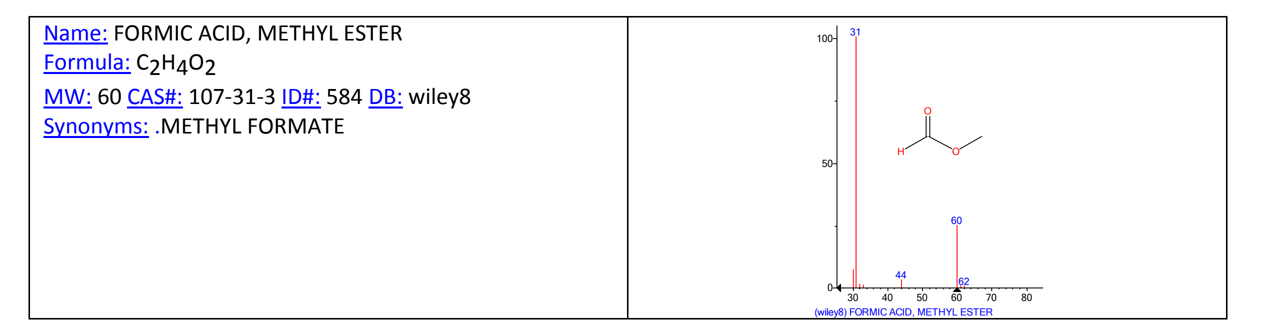
Espectros de masa de cada uno de los compuestos encontrados

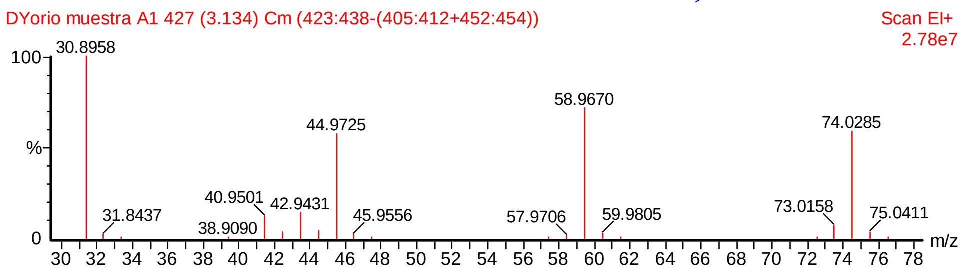
Muestra A1

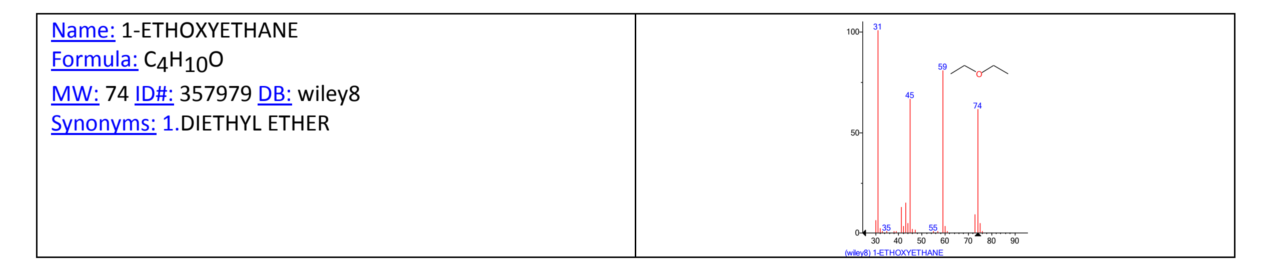












Name: 1-ETHOXYETHANE
Formula: $C_4H_{10}O$
MW: 74 ID#: 357979 DB: wiley8
Synonyms: 1.DIETHYL ETHER

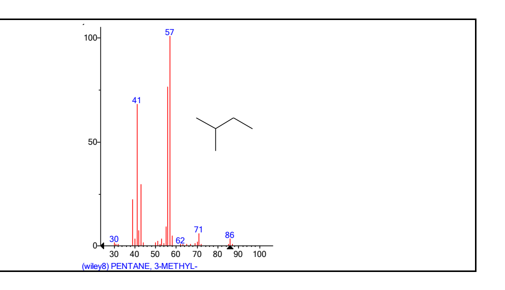
, 29-Oct-2014 + 10:33:20

DYorio muestra A1 541 (3.704) Cm (538:543-(549:554+531:537))

Scan EI+
5.82e8

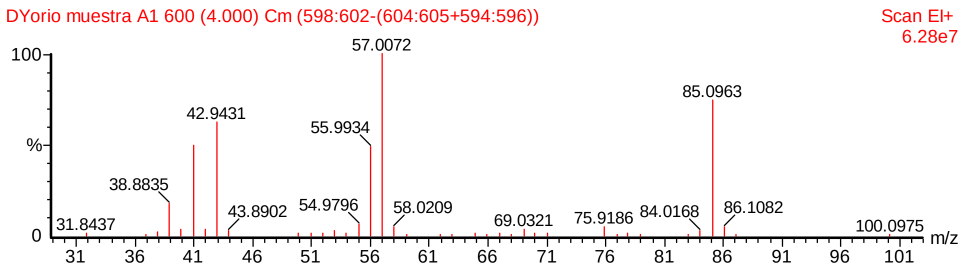
100 % 0
57.0072
40.9134
42.9431
38.8835
36.8532
50.9235
54.9796
57.9544
69.0321
71.0579
86.0408
m/z

Name: PENTANE, 3-METHYL-
Formula: C_6H_{14}
MW: 86 CAS#: 96-14-0 ID#: 3253 DB: wiley8
Synonyms: 3-METHYLPENTANE

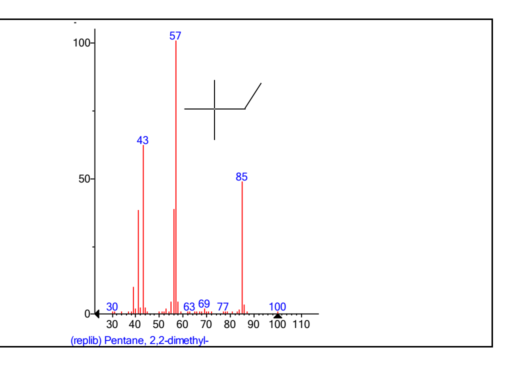


3.82 hexano

, 29-Oct-2014 + 10:33:20



Name: Pentane, 2,2-dimethyl-
Formula: C_7H_{16}
MW: 100 CAS#: 590-35-2 NIST#: 158141 ID#: 5565
Synonyms: 2,2-Dimethylpentane





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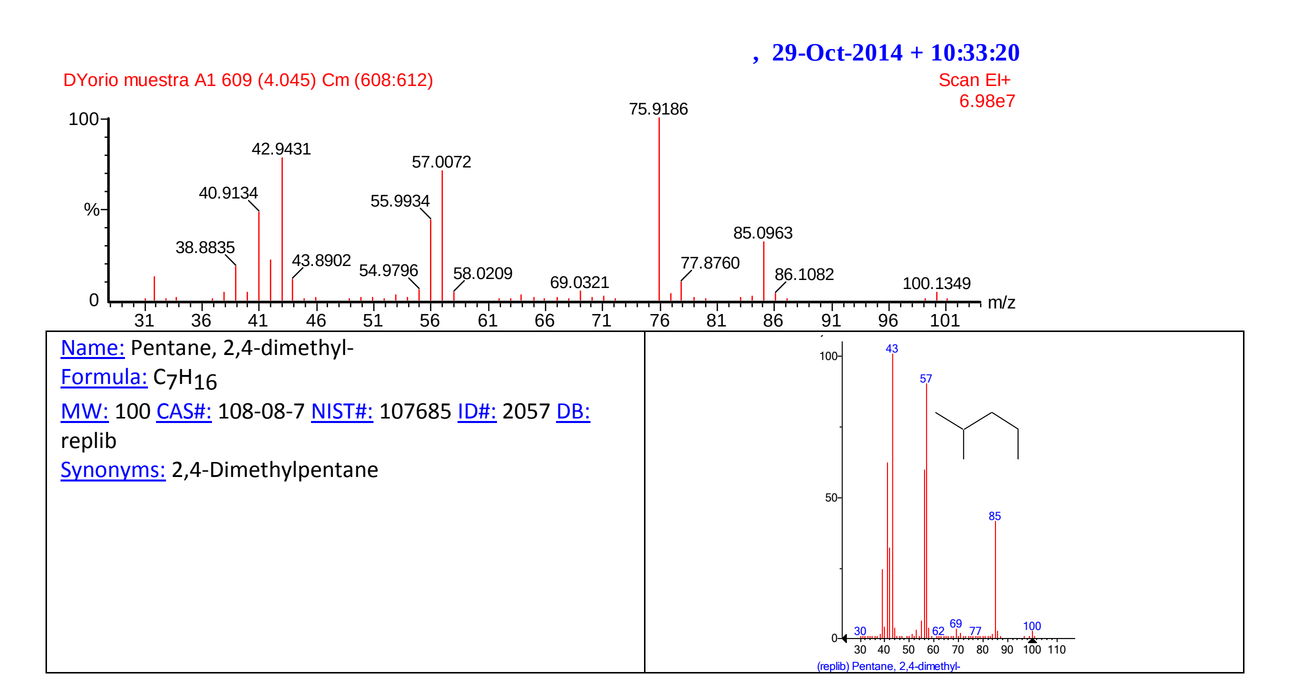
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I M B I V

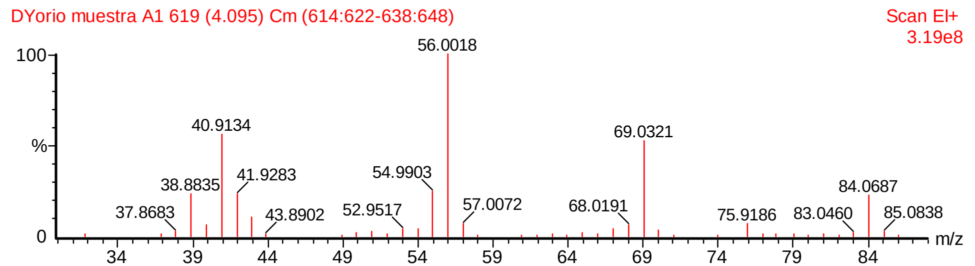
CONICET

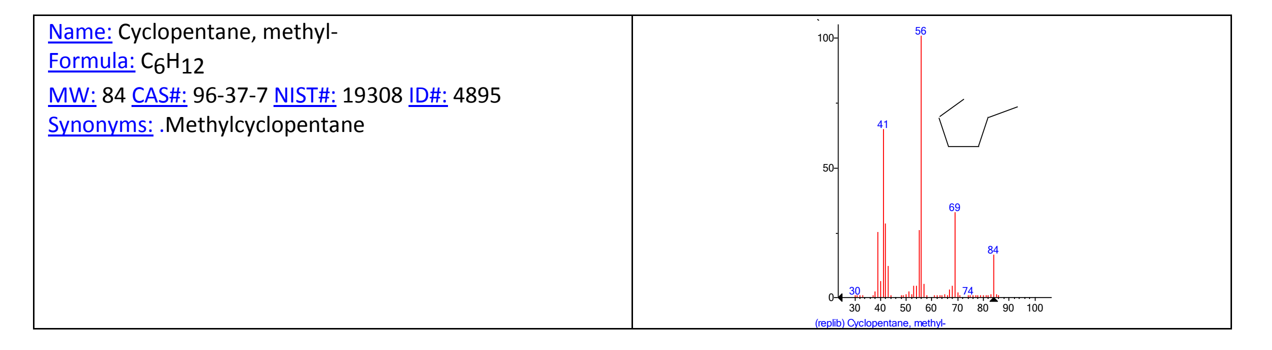
U N C

, 29-Oct-2014 + 10:33:20

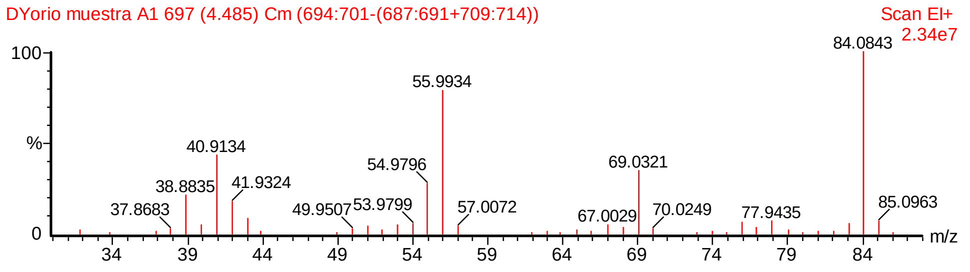








, 29-Oct-2014 + 10:33:20



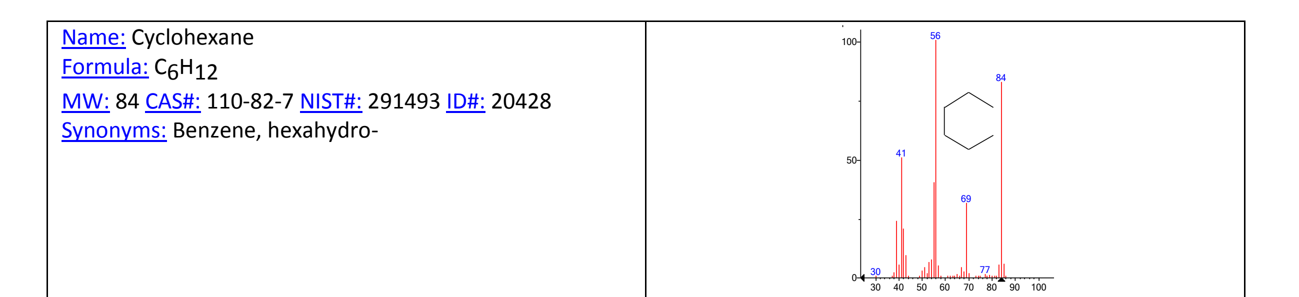
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Name: Cyclohexane
Formula: C_6H_{12}
MW: 84 CAS#: 110-82-7 NIST#: 291493 ID#: 20428
Synonyms: Benzene, hexahydro-



Muestra A2

, 29-Oct-2014 + 10:51:43

DYorio muestra A2 338 (2.689) Cm (336:340-(329:332+345:346))

Scan EI+
4.60e7

100 31.8437
%
0 32.8834 33.8748 39.8985 43.9403 m/z
31 32 33 34 35 36 37 38 39 40 41 42 43 44 45

Metanol

, 29-Oct-2014 + 10:51:43

DYorio muestra A2 349 (2.744) Cm (346:352-(359:361+343:346))

Scan EI+
2.44e6

100 59.9130
%
0 33.8737 43.8902 56.9593 61.9077 70.9583 126.9699 m/z
31 41 51 61 71 81 91 101 111 121 131

Dietileter

, 29-Oct-2014 + 10:51:43

DYorio muestra A2 425 (3.124) Cm (416:439-(404:411+446:450))

Scan EI+
1.58e7

100 30.8958
58.9670 74.0285
% 44.9725
31.8437 40.9762 42.9431 45.9838 57.9776 59.9805 73.0158 75.0399
0 m/z
30 32 34 36 38 40 42 44 46 48 50 52 54 56 58 60 62 64 66 68 70 72 74 76 78

, 29-Oct-2014 + 10:51:43

DYorio muestra A2 532 (3.659) Cm (527:535-(541:545+524:527))

Scan EI+
4.00e8

100 57.0072
40.9134
% 42.9431
38.8835 50.9235 54.9796 58.0209 69.0321 71.0579 86.0408
0 m/z
36 38 40 42 44 46 48 50 52 54 56 58 60 62 64 66 68 70 72 74 76 78 80 82 84 86 88

Metil formeato

, 29-Oct-2014 + 10:51:43
DYorio muestra A2 593 (3.965) Cm (591:594-(597:599+588))
Scan EI+
5.37e7

100
%
0
57.0072
85.0963
42.9431
56.0026
38.8835
37.8683
43.8902
54.9796
58.0209
69.0321
75.9186
84.0843
86.1082
100.1351
m/z
31 36 41 46 51 56 61 66 71 76 81 86 91 96 101

, 29-Oct-2014 + 10:51:43
DYorio muestra A2 603 (4.015) Cm (601:605-(606:607+598:599))
Scan EI+
3.37e7

100
%
0
42.9463
57.0072
40.9134
85.0963
56.0610
38.8835
31.8437
43.8902
52.9812
58.0209
71.0579
75.9186
86.1082
100.1349
m/z
32 37 42 47 52 57 62 67 72 77 82 87 92 97 102

, 29-Oct-2014 + 10:51:43
DYorio muestra A2 612 (4.060) Cm (608:614-(617:619+606:607))
Scan EI+
2.72e8

100
%
0
56.0429
40.9134
69.0321
38.8835
41.9283
55.0130
84.0843
37.8683
50.9235
52.9517
57.0072
68.0191
75.9186
83.0722
85.0963
m/z
34 39 44 49 54 59 64 69 74 79 84

, 29-Oct-2014 + 10:51:43
DYorio muestra A2 692 (4.460) Cm (688:695-(678:685+701:710))
Scan EI+
1.78e7

100
%
0
84.0843
56.0225
40.9254
55.0472
69.0321
38.8835
41.9937
37.8683
49.9769
53.9926
57.0072
67.0057
70.0461
77.9435
85.0963
m/z
34 39 44 49 54 59 64 69 74 79 84

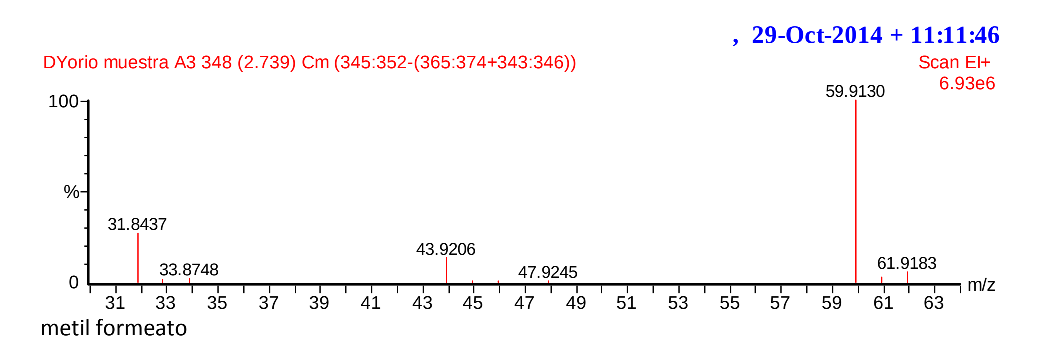
Muestra A3

, 29-Oct-2014 + 11:11:46
DYorio muestra A3 337 (2.684) Cm (334:343-(324:331+343))
Scan EI+
2.77e7

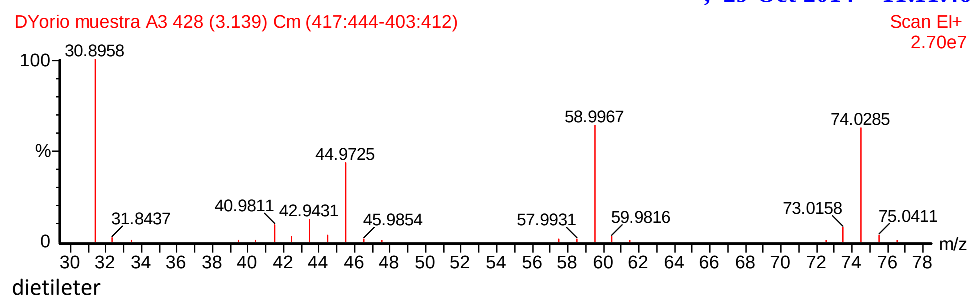
100
%
0
31.8478
43.9578
32.8819
33.8712
39.8985
44.9546
m/z
32 33 34 35 36 37 38 39 40 41 42 43 44 45 46

metanol



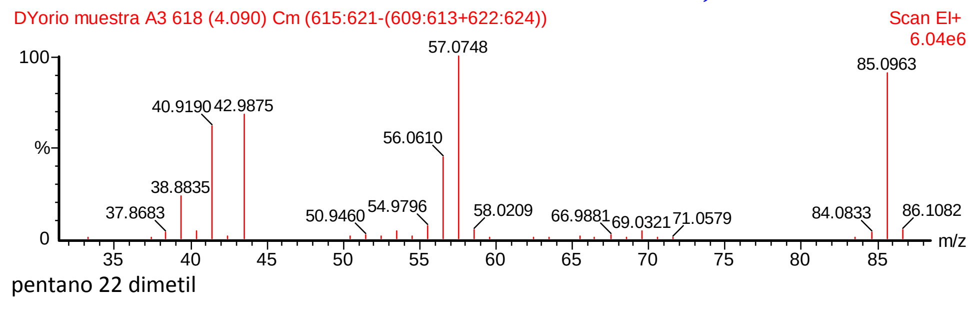


metil formeato

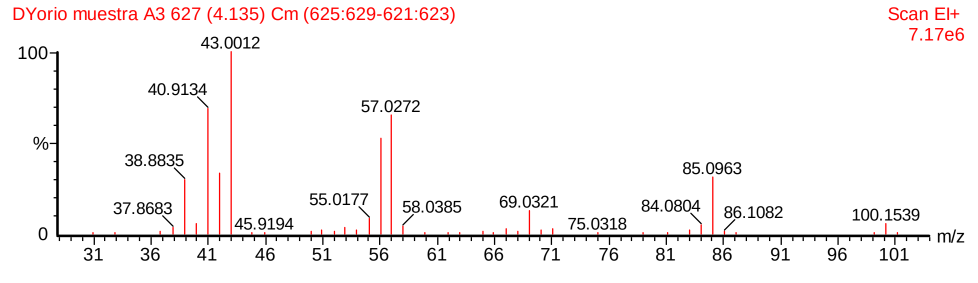


dietileter

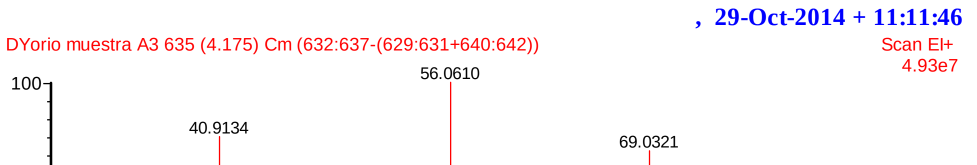
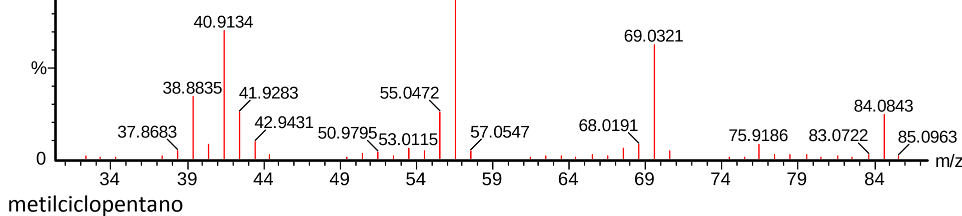
3.90 hexano



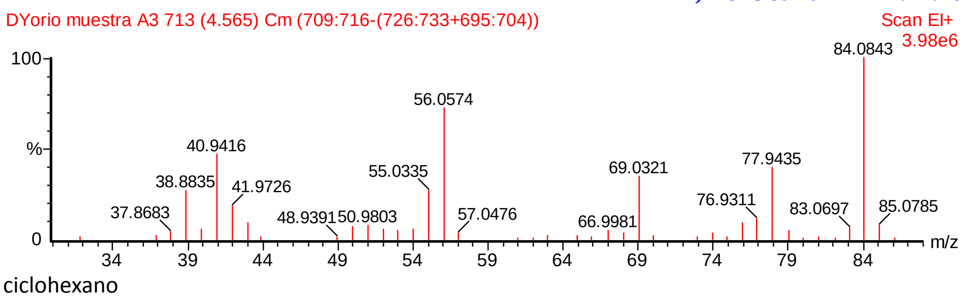
pentano 22 dimetil



Pentane, 2,4-dimethyl-

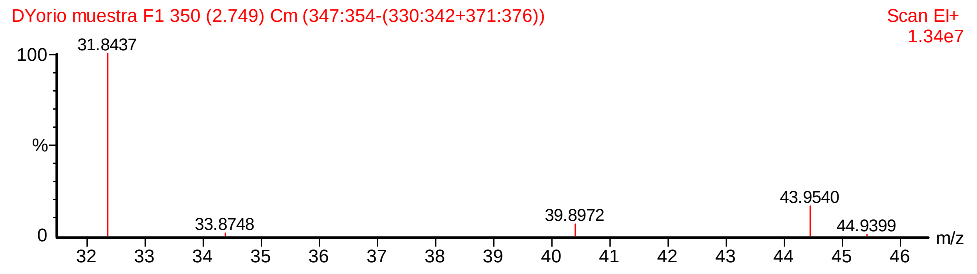



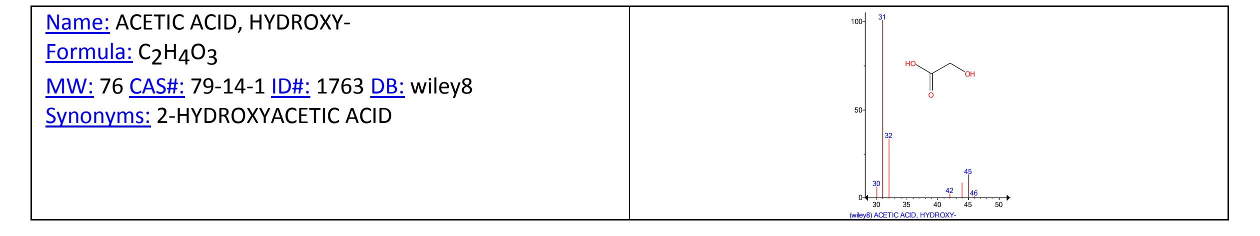
metilciclopentano



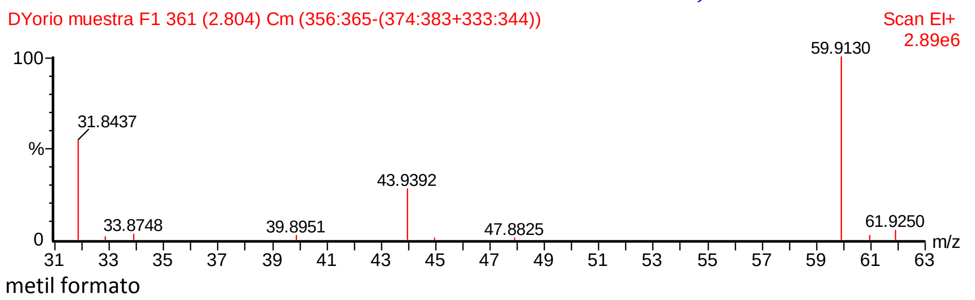
ciclohexano

Muestra F1





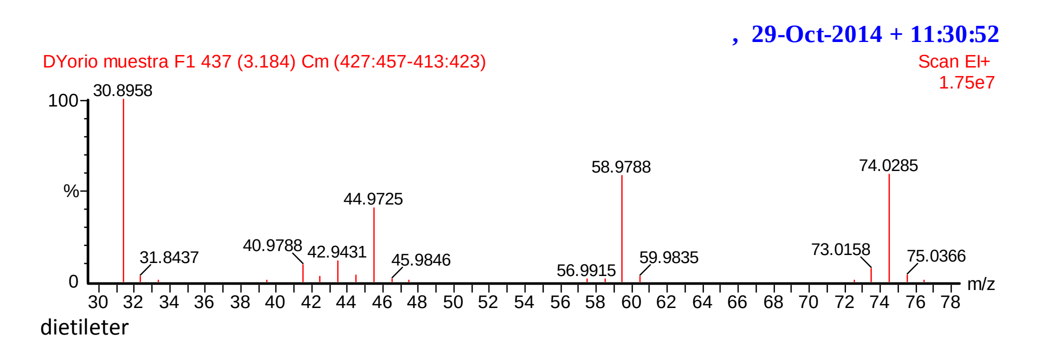
Name: ACETIC ACID, HYDROXY- Formula: $C_2H_4O_3$ MW: 76 CAS#: 79-14-1 ID#: 1763 DB: wiley8 Synonyms: 2-HYDROXYACETIC ACID	



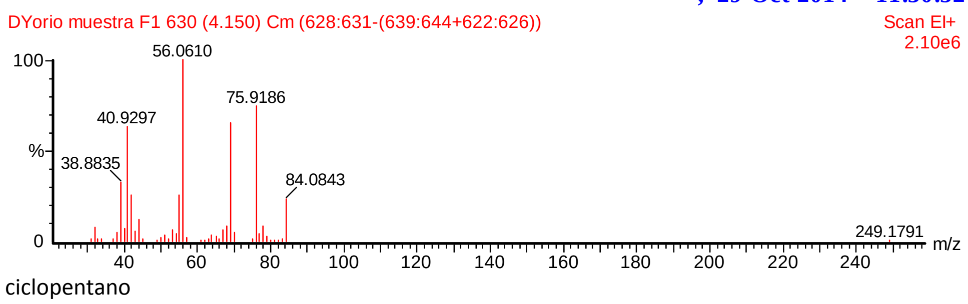
metil formato

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5000 Córdoba, Argentina
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dietileter

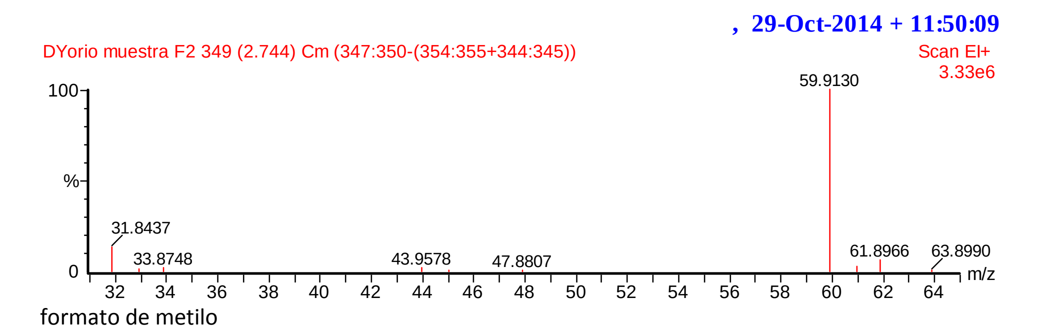


ciclopentano

Muestra F2

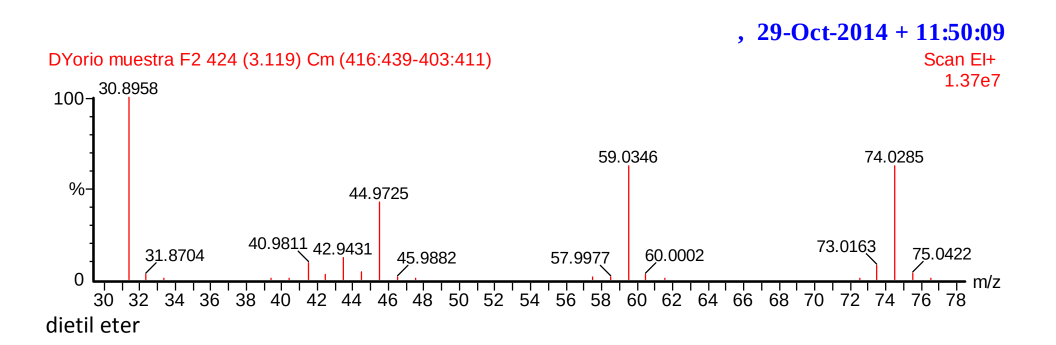
, 29-Oct-2014 + 11:50:09
DYorio muestra F2 338 (2.689) Cm (335:342-(330:333+344:346))
Scan EI+
1.65e7
100
%
0
31.8861
33.8856
39.8985
43.9578
44.9620
m/z

metanol

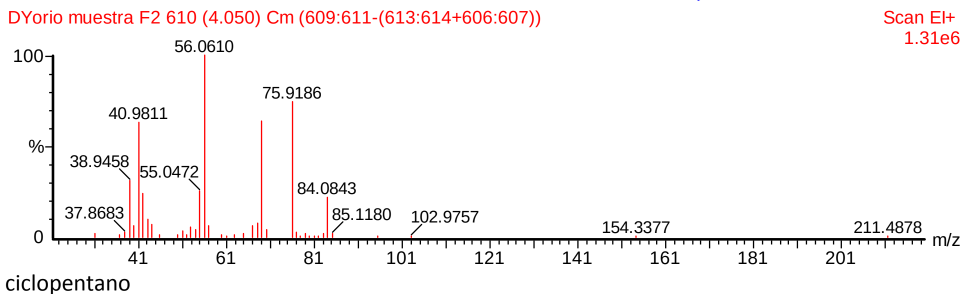


formato de metilo



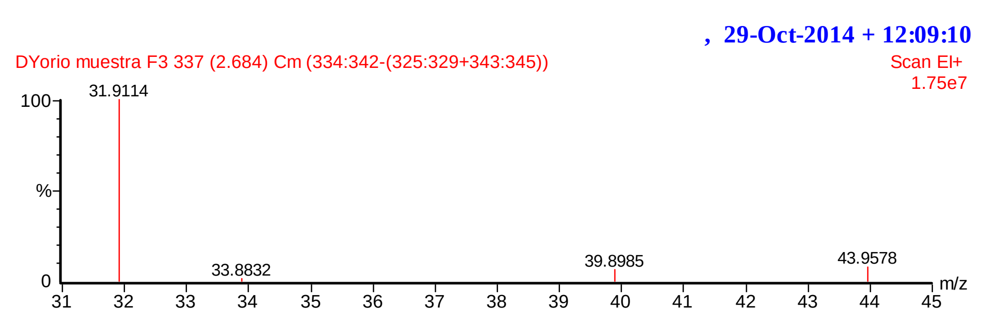


dietil eter

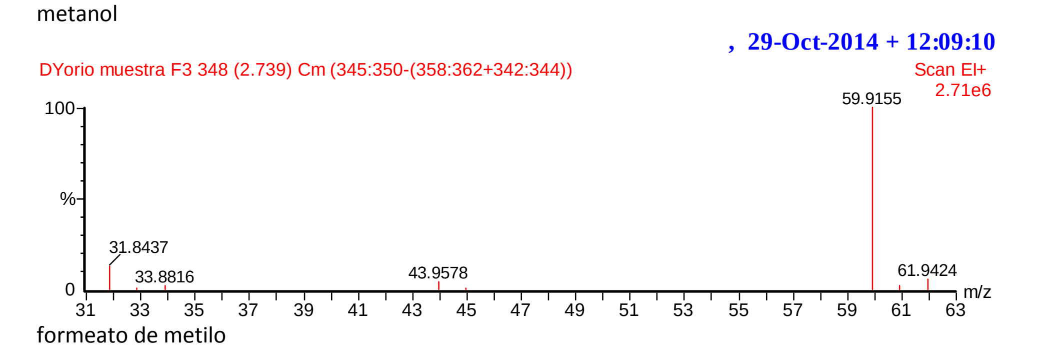


ciclopentano

Muestra F3



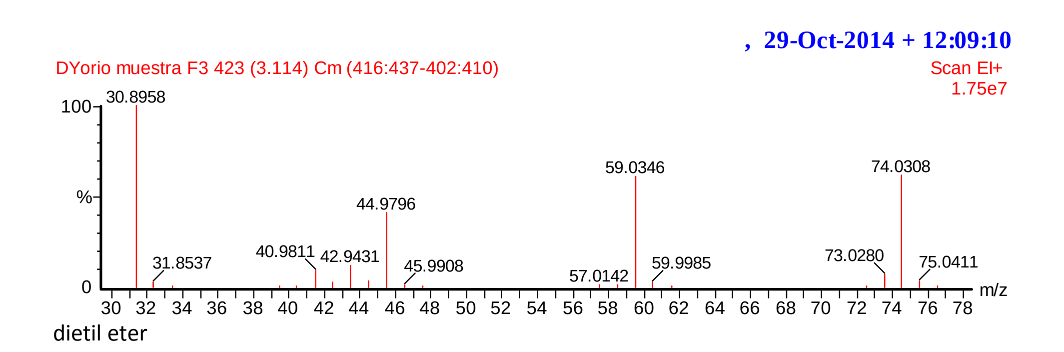
metanol



formeato de metilo

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dietil eter

OBSERVACIONES: El compuesto con tiempo de retención de 3.80 min que aparece en varios cromatogramas corresponde a hexano.


Atte., Dra. Marcela Palacio
IMBIV - Conicet – Córdoba